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(FILE 'HOME' ENTERED AT 11:17:55 ON 23 MAR 2007)  
FILE 'CA' ENTERED AT 11:19:53 ON 23 MAR 2007  
L1 365 S (THERMOCHEM? OR THERMOG? OR THERMOANALY? OR THERMAL ANALY?)AND  
(MICROARRAY OR ARRAY OR BIOCHIP OR MICROTIT? OR MICROWELL OR  
MULTIWELL OR MICROPLATE OR(96 OR 384 OR 768 OR 1536 OR 3456 OR 9600)  
(2A)WELL)  
L2 1314 S (THERMOCHEM? OR THERMOG? OR THERMOANALY? OR THERMAL ANALY?)AND  
((PHARMACEUT? OR DRUG OR MEDIC?)(2A)(SCREEN? OR TEST? OR EVALUAT? OR  
DISCOVER? OR IDENTIF? OR ASSESS? OR MONITOR?) OR COMBINATOR? OR  
HYBRIDIZ? OR MOLECU?(2A)(INTERACT? OR REACT?))  
L3 33 S L1 AND L2  
L4 29 S L1-2 AND ENZYM?  
L5 32 S L1-2 AND(96 OR 384 OR 768 OR 1536 OR 3456 OR 9600)  
L6 12 S L1-2 AND EQUILIBRAT?  
L7 24 S L1-2 AND MICROCALORIM?  
L8 177 S L1-2 AND CALORIMET?  
L9 83 S L1-2 AND INFRARED(1A)(IMAG? OR THERMOGR?)  
L10 7 S L8 AND INHIBIT?  
L11 12 S L9 AND(ENDOTHERM? OR CORRECT? OR CELL FREE OR HOTPLATE OR AGONIST)  
L12 132 S L3-7,L10-11  
L13 91 S L12 AND PY<2004  
L14 26 S L12 AND PATENT/DT  
FILE 'BIOSIS' ENTERED AT 12:14:51 ON 23 MAR 2007  
L15 24 S L13  
FILE 'MEDLINE' ENTERED AT 12:16:17 ON 23 MAR 2007  
L16 24 S L13  
FILE 'CA, BIOSIS, MEDLINE' ENTERED AT 12:18:41 ON 23 MAR 2007  
L17 117 DUP REM L13 L14 L15 L16 (48 DUPLICATES REMOVED)

=> d l17 1-117 bib,ab

L17 ANSWER 12 OF 117 CA COPYRIGHT 2007 ACS on STN  
AN 138:278132 CA  
TI Infrared spectroscopic imaging of libraries  
IN McFarland, Eric W.; Archibald, William  
PA Symyx Technologies, Inc., USA  
SO U.S., 19 pp., Cont.-in-part of U.S. 6,030,917.  
PI US 6541271 B1 20030401 US 1997-946135 19971007  
US 6030917 A 20000229 US 1997-898715 19970722  
PRAI US 1996-28105P P 19961009  
AB Methods of characterizing a relative thermal diffusivity for a plurality  
of materials are described which entail providing a thermally uniform  
substrate having a **combinatorial array** comprising a plurality of diverse  
materials at known locations on a first surface of the substrate;  
irradiating a second surface of the substrate with an IR source;  
modulating the IR source; and monitoring a temp. change assocd. with  
each of the plurality of materials as a function of time, the temp.  
change indicative of the relative thermal diffusivity of the plurality  
of materials. Systems for characterizing a relative thermal diffusivity  
for a plurality of materials are described which comprise a thermally  
uniform substrate adapted for contg. an **array** of materials on a first  
surface of the substrate; a modulated IR radiation source for directing

modulated IR radiation at a second surface of the substrate, where the IR radiation is substantially uniform across the plurality of materials; an IR detector **array** for monitoring a temp. change assocd. with each material of the plurality of materials as a function of time, the IR detector adapted for outputting a plurality of signals corresponding to the monitored temp. change for each material; and a processor coupled to the IR detector **array**, where the processor is adapted for recording the output signals from the detector **array** and detg. the relative thermal diffusivity of the plurality of materials.

L17 ANSWER 26 OF 117 CA COPYRIGHT 2007 ACS on STN

AN 137:329829 CA

TI Simultaneous high throughput assessment of thermodynamic and kinetic behaviour of chemical reactions: theory and experiment

AU Davies, Gary C.; Hutton, Roger S.; Millot, Nicolas; Macdonald, Simon J. F.; Anson, Mike S.; Campbell, Ian B.

CS GlaxoSmithKline, Harlow, Essex, CM19 5AW, UK

SO Physical Chemistry Chemical Physics (2002), 4(10), 1791-1796

AB There is an increasing requirement in the pharmaceutical industry to rapidly monitor reactions. High throughput screening (HTS) is typically achieved by performing expts. simultaneously in **array** format in **microtiter** plates. One method of monitoring reactions that has received particular attention recently is the use of thermal measurements. The change in temp. with time resulting from a reaction depends on both thermodyn. and kinetics. Temp. can be monitored in a no. of ways, one of which is suitable for HTS is **thermog.** imaging. Relating such thermal information to reaction parameters such as enthalpy and rate is complicated by issues such as heat loss to the surroundings and heat transfer to different parts of the app. A method is presented whereby information obtained from thermal imaging of **microtiter** plates can be used, along with exptl. data for heat transfer to the surroundings and the **microtiter** plate, to rank reaction enthalpy and time to completion of a set of reactions. Finally, a comparison to enthalpies obtained by **microcalorimetry** is made.

L17 ANSWER 28 OF 117 CA COPYRIGHT 2007 ACS on STN

AN 137:41018 CA

TI Rapid determination of enantiomeric excess using infrared **thermography**

AU Millot, Nicolas; Borman, Phil; Anson, Mike S.; Campbell, Ian B.; Macdonald, Simon J. F.; Mahmoudian, Mahmoud

CS Medicines Research Centre, GlaxoSmithKline Research and Development, Hertfordshire, SG1 2NY, UK

SO Organic Process Research & Development (2002), 6(4), 463-470

AB IR **thermog.** (IRT) is presented as a novel technique to screen a potentially large no. of asym. catalysts or substrates in a high-throughput fashion. IRT was used as a simple, rapid, and practical approach for initial screening of the substrate specificity of *Candida antarctica* lipase. This was carried out using a **96-well microtiter** plate format. Potential advantages and limitations of IRT for the **enzymic** stereoselective acylation of primary and secondary alcs. of interest are discussed.

L17 ANSWER 35 OF 117 CA COPYRIGHT 2007 ACS on STN

AN 134:125924 CA  
 TI **Thermochemical** sensors and use in **pharmaceutical** agent **screening**  
 IN Connelly, Patrick R.; Ali, Janid Asghar; Bruzzese, Frank Joseph;  
 Faerman, Carlos H.  
 PA The Althexis Co., Inc., USA  
 SO PCT Int. Appl., 98 pp.  
 PI WO 2001006250 A2 20010125 WO 2000-US19383 20000718  
 PRAI US 1999-144579P P 19990719  
 AB Methods are provided to link the binding event of a test ligand or  
 substrate to a target (e.g. a target protein) to the generation of a  
 heat output. The methods can be used to **screen** for **pharmaceutical**  
 agents.

L17 ANSWER 40 OF 117 CA COPYRIGHT 2007 ACS on STN  
 AN 135:163919 CA  
 TI Infrared-**thermographic** screening of the activity and enantioselectivity  
 of **enzymes**  
 AU Reetz, M. T.; Hermes, M.; Becker, M. H.  
 CS Max-Planck-Institut fur Kohlenforschung, Mulheim an der Ruhr, 45470,  
 Germany  
 SO Applied Microbiology and Biotechnology (2001), 55(5), 531-536  
 AB A review with approx. 50 refs. The IR radiation caused by the heat of  
 reaction of an enantioselective **enzyme**-catalyzed transformation can be  
 detected by modern photovoltaic IR (IR)-**thermog.** cameras equipped with  
 focal plane **array** detectors. Specifically, in the lipase-catalyzed  
 enantioselective acylation of racemic 1-phenylethanol, the (R)- and (S)-  
 substrates are allowed to react sep. in the wells of **microtiter** plates,  
 the (R)-alc. showing hot spots in the IR-**thermog.** images. Thus, highly  
 enantioselective **enzymes** can be identified at kinetic resolu.

L17 ANSWER 43 OF 117 MEDLINE on STN  
 AN 2001354994 MEDLINE  
 TI Novel methods for biocatalyst screening.  
 AU Wahler D; Reymond J L  
 CS Departement fur Chemie und Biochemie, Universitat Bern, Switzerland.  
 SO Current opinion in chemical biology, (2001 Apr) Vol. 5, No. 2, pp. 152-  
 8.  
 AB There have been a number of recent advances in catalysis assays  
 applicable for screening biocatalyst libraries in high-throughput  
 format. These include instrumental assays such as high-performance  
 liquid chromatography, mass spectrometry, capillary electrophoresis and  
 IR-**thermography**, reagent-based assays producing spectroscopic signals  
 (UV/VIS or fluorescence) in response to reaction progress, and assays  
 based on fluorogenic or chromogenic substrates. These fluorogenic  
 substrates enable the assaying of a variety of **enzymes** in  
 enantioselective and stereoselective manner, including alcohol  
 dehydrogenases, aldolases, lipases, amidases, epoxide hydrolases and  
 phosphatases.

L17 ANSWER 51 OF 117 CA COPYRIGHT 2007 ACS on STN  
 AN 133:266394 CA  
 TI **IR-thermographic** screening of thermoneutral or **endothermic**  
 transformations: the ring-closing olefin metathesis reaction

AU Reetz, Manfred T.; Becker, Michael H.; Liebl, Monika; Furstner, Alois  
 CS Max-Planck-Institut fur Kohlenforschung, Mulheim an der Ruhr, 45470, Germany  
 SO Angewandte Chemie, International Edition (2000), 39(7), 1236-1239  
 AB In appropriate systems **endothermic** or even thermoneutral reactions can be successfully screened by resolved detection of cold spots in **IR-thermog. images**. This is useful for screening **combinatorial** libraries of catalysts.

L17 ANSWER 54 OF 117 CA COPYRIGHT 2007 ACS on STN  
 AN 132:227998 CA  
 TI Catalytic phenomena in **combinatorial** libraries of heterogeneous catalysts detection of activation and deactivation by emissivity-corrected **IR thermography**  
 AU Holzwarth, Arnold; Maier, Wilhelm F.  
 CS Max-Planck-Institut fur Kohlenforschung, Mulheim an der Ruhr, Germany  
 SO Platinum Metals Review (2000), 44(1), 16-21  
 AB A review with 13 refs.; **combinatorial** catalysis is becoming a significant method for investigating the activities of large nos. of potential catalysts. A very important prerequisite for making use of **combinatorial** catalysis research is a reliable, fast and efficient technique for monitoring the catalytic activities. Emissivity-cor. **IR thermog.**, which monitors the heat changes resulting from the heat of reaction on catalyst surfaces, is such a technique. In this article we describe emissivity-cor. **IR thermog.** and demonstrate its performance, over time, in monitoring the catalytic activities of catalyst libraries. It is shown that not only can static relative activity be displayed, but also that catalyst-specific time-dependent properties, such as activation and deactivation phenomena can be demonstrated.

L17 ANSWER 55 OF 117 CA COPYRIGHT 2007 ACS on STN  
 AN 132:1820 CA  
 TI **Infrared thermography** for measuring real-time **thermogenesis** in organisms and cells  
 IN Lenhard, James Martin; Paulik, Mark Andrew  
 PA Glaxo Group Limited, UK  
 SO PCT Int. Appl., 93 pp.  
 PI WO 9960630 A1 19991125 WO 1999-US10579 19990514  
 US 6881584 B1 20050419 US 1999-441493 19991117  
 PRAI US 1998-85736P P 19980515  
 AB The present invention relates, in general, to **thermog.** and, in particular, to a method of using **IR thermog.** to monitor physiol. and mol. events that elicit a **thermogenic** response in animals (including humans), plants, tissues, cells and **cell-free** systems. The present method can be used for screening, **identifying**, and ranking **drug** candidates for multiple diseases, disorders and conditions. Three different inbred strains of mice, AKR/J, C57BL/6J, and SWR/J, were maintained on high and low fat diets for 14 wk before treatment with the  $\beta$ 3-adrenoceptor **agonist**, BRL37344. The heat produced in the intrascapular region was measured before and after 60 min treatment using **IR thermog.** The obesity prone mice, AKR/J, had a greater **thermogenic** response to BRL37344 when fed the higher fat diet. The

obesity resistant mice, SWR/J, had a greater **thermogenic** response when fed the lower fat diet. There was little difference in the response of C57BL/6J mice on a high or low fat diet.

L17 ANSWER 67 OF 117 CA COPYRIGHT 2007 ACS on STN  
AN 130:95129 CA  
TI Time-resolved IR-**thermographic** detection and screening of enantioselectivity in catalytic reactions  
AU Reetz, Manfred T.; Becker, Michael H.; Kuhling, Klaus M.; Holzwarth, Arnold  
CS Max-Planck-Institut fur Kohlenforschung, Mulheim an der Ruhr, D-45470, Germany  
SO Angewandte Chemie, International Edition (1998), 37(19), 2647-2650  
AB Time-resolved IR **thermog.** was applied to screening of enantioselectivity in catalytic reactions,. Since spacial resoln. is not a problem, the screening of large libraries of asym. catalysts could be possible. The method could also be amenable co other chem. or biochem. processes such as mol. recognition in host-guest chem. or antibody-antigen interactions.  
RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 68 OF 117 CA COPYRIGHT 2007 ACS on STN  
AN 129:307011 CA  
TI Detection of catalytic activity in **combinatorial** libraries of heterogeneous catalysts by **IR thermography**  
AU Holzwarth, Arnold; Schmidt, Hans-Werner; Maier, Wilhelm F.  
CS Max-Planck-Institut fur Kohlenforschung, Mulheim an der Ruhr, D-45470, Germany  
SO Angewandte Chemie, International Edition (1998), 37(19), 2644-2647  
AB The primary interest of this study was to display temp. differences due to catalytic activity on a library of heterogeneous catalysts. This was achieved by applying a linear **correction** to the detector response and subtracting the **IR image** of the library just before the start of the reaction as background (offset) from the images during an isothermal catalytic expt. We have demonstrated that, after careful removal of artifacts, **IR imaging** is a powerful tool for the detection of catalytic activities on **combinatorial** libraries. Temp. differences down to 0.1 K can reliably be detected and the heat evolution of catalyzed gas-phase reactions on small catalyst amts. (<20 $\mu$ g) identified. Reactions have been obsd. at temps. up to 350°C, indicating that the method can be applied over a wide temp. range.

L17 ANSWER 69 OF 117 CA COPYRIGHT 2007 ACS on STN  
AN 129:117364 CA  
TI Development of **infrared imaging** to measure **thermogenesis** in cell culture: **thermogenic** effects of uncoupling protein-2, troglitazone, and  $\beta$ -adrenoceptor **agonists**  
AU Paulik, Mark A.; Buckholz, Richard G.; Lancaster, Mary E.; Dallas, Walter S.; Hull-Ryde, Emily A.; Weiel, James E.; Lenhard, James M.  
CS Department of Metabolic Diseases, GlaxoWellcome Inc. Research Triangle Park, NC, 27709, USA  
SO Pharmaceutical Research (1998), 15(6), 944-949

AB Although the effects of **thermogenic** agents in cell culture can be measured by direct **microcalorimetry**, only a few samples can be analyzed over several hours. In this report, we describe a robust non-invasive technique to measure real-time **thermogenesis** of cells cultured in **microtiter** plates using IR **thermog.** Yeast were transformed with uncoupling protein-2 (UCP2) or exposed to carbonyl cyanide p-(trifluoromethoxy)phenylhydrazone (FCCP) or rotenone. Adipocytes were exposed to rotenone, FCCP, cycloheximide, troglitazone, or CL316243. **Thermogenesis** was measured using IR **thermog.** **Thermogenesis** increased after exposing yeast to the mitochondrial uncoupler, FCCP, or transforming the cells with UCP2. Further, **thermogenesis** in adipocytes was stimulated by CL316243, a  $\beta$ 3-adrenoceptor **agonist** being developed to treat obesity. The protein synthesis inhibitor, cycloheximide, did not inhibit CL316243-mediated **thermogenesis**. In contrast, the mitochondrial proton transport inhibitor, rotenone, inhibited **thermogenesis** in yeast and adipocytes. Similarly, the antidiabetic agent, troglitazone, suppressed **thermogenesis** in adipocytes. Although increased UCP synthesis resulted in increased **thermogenesis** in yeast, UCP expression did not correlated with **thermogenesis** in adipocytes. The results, taken together with the high resoln. (0.002°C) and robustness (**384-well** format) of the approach, indicate **IR-imaging** is a rapid and effective method for measuring **thermogenesis** in vitro.

L17 ANSWER 77 OF 117 CA COPYRIGHT 2007 ACS on STN

AN 127:250453 CA

TI Catalyst testing process and apparatus

IN Willson, Richard Coale, III

PA Technology Licensing Co. L.L.C., USA; Willson, Richard Coale, III

SO PCT Int. Appl., 35 pp.

PI WO 9732208 A1 19970904 WO 1997-US2756 19970225

US 6063633 A 20000516 US 1996-664836 19960617

PRAI US 1996-12457P P 19960228

AB A multicell holder, e.g., a honeycomb or plate, or a collection of individual support particles, is treated with solns./suspensions of catalyst ingredients to produce a plurality of cells, spots, or pellets each having a different compn. The plurality of cells, spots, or pellets are dried, calcined or treated to stabilize the ingredients and contacted with a potentially reactive feed stream or batch of reactants. The reaction occurring in each cell is measured or analyzed to det. the relative efficacy of the catalysts in each combination. The measurement or anal. is done through a no. of different methods including IR **thermog.**, spectroscopy of products or residual reactants or sampling for further anal. Robotic techniques can be employed in producing the cells, spots or pellets.

L17 ANSWER 96 OF 117 CA COPYRIGHT 2007 ACS on STN

AN 119:240815 CA

TI Application of **microcalorimetric** technique for the screening and examination of medicines

AU Zhang, Youmin; Wang, Baohuai

CS Inst. Phys. Chem., Beijing Univ., Beijing, 100871, Peop. Rep. China

SO Journal of Chinese Pharmaceutical Sciences (1993), 2(1), 24-32

AB According to the heating effect caused by interaction between matters, a

series of expts. on the interaction between drugs and cells from human bodies, DNA and physiol. saline have been carried out with MS-80 std. Calvet **microcalorimeter**. The expts. include: (1) thermokinetic studies of the effect of anticancer drugs [sodium norcantharidate (ASN), the bioactive material (Sp.P and Sp.S) from algae etc.] on cancer cells [Hela, human breast carcinoma Bcap-37), human adenocarcinoma gastric cells (SGC-7901 and MCF-7) etc.] and the normal cells from human bodies [diploid fibroblasts from human fetal lung (2BS) etc.] at 310.15 K; (2) studies of the intercalation binding of some alkaloidal drugs with the bioactivity to **inhibit** monoamine oxidase (harmaline and harmine etc.) to calf thymus DNA in neutral aq. soln. at 298.15 K; (3) studied of the interaction between long acting drugs (long acting oral contraceptive-norgestrel etc.) and slow-releasing drug (Contac) and aq. soln. of 0.9% NaCl at 310.15 K. All the exptl. results have given their characteristic **thermograms** and the interaction enthalpy changes. On the anal. of all the results, the authors put forward a method on application of **microcalorimetric** technique for screening and examn. of medicines. The principle of application and the exptl. operation of this method have been expounded, and some results of the above expts. have been discussed. As one of the methods for **screening** and examg. **medicines**, the **microcalorimetric** method has some distinguished features and advantages over other methods.

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STN INTERNATIONAL LOGOFF AT 12:19:49 ON 23 MAR 2007